Species	$K_{H\ 298,}$ [M atm-1]	-ΔH/R, [K]	α	$D_{g\ 298}$, [105 m^2 s^{-1}]
aCO2	3.10E-02	2423.0	1.50E-04	1.55
aO3	1.14E-02	2300.0	0.1	1.48
aHO2	9.00E+03		1.00E-02	1.04
aHO	2.50E+01	5280.0	5.00E-02	1.53
aH2O2	1.02E+05	6340.0	1.532E-01	1.46
aNO2	1.20E-02	1263.0	1.50E-03	1.92
aHONO	4.90E+01	4880.0	5.00E-02	1.3
aHNO3	2.10E+05	8700.0	8.68E-02	1.32
aNO3	6.00E-01		4.00E-03	1.0
aN2O5	1.40E+00		1.80E-02	1.1
aNH3	6.07E+01	3920.0	9.10E-02	2.3
aHCL	1.10E+00	2020.0	1.158E-01	1.89
aHCHO	2.50E+00	7216.0	2.00E-02	1.64
aORA1	5.53E+03	5630.0	2.29E-02	1.53
aSO2	1.24E+00	3247.0	1.10E-01	1.28
aOP1	3.10E+02	5607.0	6.7581E-03	1.31

Species	$K_{H\ 298,}$ [M atm-1]	-ΔH/R, [K]	α	$D_{g\ 298}$, [105 m^2 s^{-1}]
aCH3COOH	5.50E+03	5890.0	3.22E-02	1.24
aPAA	6.69E+02	5890.0	1.90E-02	1.02
aMO2	3.10E+02	5607.0	6.7581E-03	1.35
aETHPX	3.40E+02	87.0	8.20E-03	1.08
aETOH	1.90E+02	6290.0	1.76E-02	0.95
aCH3OH	2.20E+02	5390.0	2.71E-02	1.16
aCH3CHO	4.80E+00	6254.0	3.00E-02	1.22
aBR2	7.60E-01	4100.0	8.00E-02	1.0
aCL2	9.15E-02	2490.0	8.00E-02	1.28
aSULF	8.70E+11		1.20E-01	1.3
aHNO4	3.00E+04		0.1	1.3
aACO3	6.69E+02	5893.0	1.90E-02	1.0
aCHOH2CHOH2	3.03E+05		2.30E-02	1.15
aO2	1.30E-03	1700.0	0.1	1.12
aCLNO2	2.40E-02		1.00E-02	1.44

Species	$K_{H\ 298,}$ [M atm-1]	-ΔH/R, [K]	α	$D_{g\ 298}$, [105 m^2 s^{-1}]
aBRNO2	3.00E-01		1.00E-02	1.44
aNO	1.90E-03	1400.0	1.00E-03	2.24
aC2H5CHO	1.30E+01	5700.0	3.00E-02	1.0
aCH3CH2CH2CHO	9.60E+00	6200.0	3.00E-02	0.87
aCH3CH2COOH	5.71E+03		3.22E-02	0.93
aCH3CH2CH2COOH	4.70E+03		3.00E-02	0.82
aCH3COCHOH2	3.78E+03	7541.0	3.00E-02	0.95
aOHCCHCHCHO	3.00E+05		2.30E-02	0.86
aCH2OHCH2OH	4.00E+06		4.00E-02	1.06
aOHCCH2OH	4.10E+03	4630.5	4.00E-02	1.1

Table A2. Aqueous phase processes in C3.0RED. Comments indicates the “origin" of the selected aqueous processes that are considered in the final reduced mechanism based on the manual (MR) and automatic (AR) mechanism reduction.

A- Aqueous phase reactions:

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Comment
		HO_x- and Transition metal ion (TMI)-Chemistry			
R1	R1†*	$H_2O_2 + Fe^{2+} \rightarrow OH + OH^- + Fe^{3+}$	50		
R2	R2*	$Mn(OH)^{2+} + H_2O_2 \rightarrow MnO_2^+ + H^+ + H_2O$	$2.8 \cdot 10^3$		Implemented based on the ISSA studies (AR)
R3	R4†*	$H_2O_2 + Cu^+ \rightarrow OH + OH^- + Cu^{2+}$	$7.0 \cdot 10^3$		
R4	R6†*	$O_2^- + Fe^{3+} \rightarrow O_2 + Fe^{2+}$	$1.5 \cdot 10^8$		
	R7†	$HO_2 + [Fe(OH)]^{2+} \rightarrow Fe^{2+} + O_2 + H_2O$	$1.3 \cdot 10^5$		Removed based on the ISSA studies (AR), $k(HO_2) << k(O_2^-)$)
R5	R8†*	$O_2^- + [Fe(OH)]^{2+} \rightarrow O_2 + Fe^{2+} + OH^-$	$1.5 \cdot 10^8$		
R6	R10†*	$O_2^- + Fe^{2+} (+ 2\ H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.0 \cdot 10^7$		
R7	R11†*	$HO_2 + Fe^{2+} (+ H^+) \rightarrow H_2O_2 + Fe^{3+}$	$1.2 \cdot 10^6$	5050	
	R12†	$OH + Fe^{2+} \rightarrow [Fe(OH)]^{2+}$	$4.3 \cdot 10^8$	1100	Removed based on the ISSA studies (AR)
R8	R13*	$MnO_2^+ + HO_2 (+ H^+) \rightarrow Mn^{2+} + H_2O_2 + O_2$	$1 \cdot 10^7$		Implemented based on the ISSA studies (AR)
R9	R15†*	$O_2^- + Cu^+ (+ 2\ H^+) \rightarrow H_2O_2 + Cu^{2+}$	$1 \cdot 10^{10}$		
R10	R16†*	$HO_2 + Cu^+ (+ H^+) \rightarrow H_2O_2 + Cu^{2+}$	$2.3 \cdot 10^9$		
R11	R18†*	$HO_2 + Cu^{2+} \rightarrow O_2 + Cu^+ + H^+$	$1 \cdot 10^8$		
R12	R19†*	$O_2^- + Cu^{2+} \rightarrow O_2 + Cu^+$	$8 \cdot 10^9$		
R13	R20†*	$Fe^{3+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+}$	$1.3 \cdot 10^7$		
R14	R21†*	$[Fe(OH)]^{2+} + Cu^+ \rightarrow Fe^{2+} + Cu^{2+} + OH^-$	$1.3 \cdot 10^7$		
R15	R24†*	$O_3 + O_2^- \rightarrow O_3^- + O_2$	$1.5 \cdot 10^9$	2200	
R16	R25†*	$HO_3 \rightarrow OH + O_2$	330	4500	
R17	R30†*	$H_2O_2 + OH \rightarrow HO_2 + H_2O$	$3.0 \cdot 10^7$	1680	
R18	R33†	$HSO_3^- + OH \rightarrow H_2O + SO_3^-$	$2.7 \cdot 10^9$		Implemented based on the non-permanent cloud MR studies (important SO_4^- sink) (due to the high pK_{a2} value of 7.22)
R19	R34*	$SO_3^{2-} + OH \rightarrow OH^- + SO_3^-$	$4.6 \cdot 10^9$		Implemented based on the ISSA studies (AR)

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n}\ s^{-1}$	E_a / R, K	Comment
R20	R36†*	$Cu^{+} + O_2 \rightarrow Cu^{2+} + O_2^{-}$	$4.6 \cdot 10^5$		
R21	R37†*	$Fe^{2+} + O_3 \rightarrow FeO^{2+} + O_2$	$8.2 \cdot 10^5$	4690	
R22	R38*	$FeO^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO_2 + OH^{-}$	$9.5 \cdot 10^3$	2766	Implemented based on the ISSA studies (AR)
R23	R43*	$FeO^{2+} + HSO_3^{-} \rightarrow Fe^{3+} + SO_3^{-} + OH^{-}$	$2.5 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R24	R47*	$FeO^{2+} + HCOO^{-} (+ H^{+}) \rightarrow Fe^{3+} + COOH + OH^{-}$	$3 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R25	R44†*	$FeO^{2+} + Cl^{-} (+ H^{+}) \rightarrow Fe^{3+} + ClOH^{-}$	100		
R26	R51†*	$FeO^{2+} + Fe^{2+} \rightarrow 2\ Fe^{3+} + 2\ OH^{-}$	$7.2 \cdot 10^4$	842	
R27	R52*	$FeO^{2+} + Fe^{2+} (+ H_2O) \rightarrow FeOH_2Fe^{4+}$	$1.8 \cdot 10^4$	5052	Implemented based on the ISSA studies (AR)
R28	R54*	$FeOH_2Fe^{4+} \rightarrow 2\ Fe^{3+} + 2\ OH^{-}$	0.49	8780	Implemented based on the ISSA studies (AR)
R29	R55*	$MnO^{2+} + Mn^{2+} (+ 2\ H^{+}) \rightarrow 2\ Mn^{3+} + H_2O$	$1 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R30	R56*	$Mn^{2+} + O_3 \rightarrow MnO^{2+} + O_2$	$1.65 \cdot 10^3$		Implemented based on the ISSA studies (AR)
		Nitrogen-Chemistry			
R31	R60†*	$N_2O_5 \rightarrow NO_2^{+} + NO_3^{-}$	$1 \cdot 10^9$		
R32	R61†*	$NO_2^{+} + H_2O \rightarrow NO_3^{-} + 2H^{+}$	$8.9 \cdot 10^7$		
R33	R65†*	$NO_3 + H_2O_2 \rightarrow NO_3^{-} + H^{+} + HO_2$	$4.9 \cdot 10^6$	2000	
R34	R69†	$NO_3 + HSO_3^{-} \rightarrow NO_3^{-} + H^{+} + SO_3^{-}$	$1.3 \cdot 10^9$	2000	Implemented based on the non-permanent modelling: Important inorganic NO_3 sink under urban conditions
R35	R71*	$NO_3 + HSO_4^{-} \rightarrow NO_3^{-} + H^{+} + SO_4^{-}$	$2.6 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R36	R72†*	$NO_3 + SO_4^{2-} \rightarrow NO_3^{-} + SO_4^{-}$	$1 \cdot 10^5$		
R37	R76†*	$O_2NO_2^{-} \rightarrow NO_2^{-} + O_2$	$4.5 \cdot 10^{-2}$		
	R85†	$NO_2^{+} + Cl^{-} \rightarrow ClNO_2$	$1 \cdot 10^{10}$		Removed based on the ISSA studies (AR)
		Sulphur-Chemistry			
	R90†	$HMS^{-} + OH \rightarrow H_2O + CHOHSO_3^{-}$	$3 \cdot 10^8$		Removed based on the non-permanent cloud studies (MR)
	R97†	$CHOHSO_3^{-} + O_2 \rightarrow O_2CHOHSO_3^{-}$	$2.6 \cdot 10^9$		Removed based on the non-permanent cloud studies (MR)
	R98†	$O_2CHOHSO_3^{-} \rightarrow HO_2 + CHOSO_3^{-}$	$1.7 \cdot 10^4$		Removed based on the non-permanent cloud studies (MR)
	R99†	$O_2CHOHSO_3^{-} \rightarrow O_2CHO + HSO_3^{-}$	$7.0 \cdot 10^3$		Removed based on the non-permanent cloud studies (MR)

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n} s^{-1}$	E_a / R, K	Comment
	R100†	$CHOSO_3^- + H_2O \rightarrow HSO_3^- + HCOOH$	$1.26 \cdot 10^{-2}$		Removed based on the non-permanent cloud studies (MR)
	R101†	$O_2CHO + H_2O \rightarrow HCOOH + HO2$	44.32		Removed based on the non-permanent cloud studies (MR)
	R102†	$CHOSO_3^{2-} + O_2 \rightarrow CHOSO_3^- + O_2^-$	$1.6 \cdot 10^9$		Removed based on the non-permanent cloud studies (MR)
R38	R103†*	$HSO_3^- + H_2O_2 + H^+ \rightarrow SO_4^{2-} + H_2O + 2\ H^+$	$7.2 \cdot 10^7$	4000	
R39	R104	$HSO_3^- + CH_3OOH + H^+ \rightarrow SO_4^{2-} + 2\ H^+ + CH_3OH$	$1.7 \cdot 10^7$	3800	CH_3OOH treatment implemented based on the non-permanent modelling: Most important organic S(VI) formation pathway
R40	R105*	$HSO_3^- + CH_3C(O)OOH + H^+ \rightarrow SO_4^{2-} + 2\ H^+ + CH_3COOH$	$5.6 \cdot 10^7$	3990	Implemented based on the ISSA studies (AR)
	R107†	$HSO_3^- + O_3 \rightarrow HSO_4^- + O_2$	$3.7 \cdot 10^5$	5530	Removed based on the ISSA studies (AR) ($k_{HSO3-} << k_{SO32-}$)
R41	R108†*	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-} + O_2$	$1.5 \cdot 10^9$	5280	
R42	R110†*	$Fe^{2+} + SO_5^- (+ H_2O) \rightarrow [Fe(OH)]^{2+} + HSO_5^-$	$2.65 \cdot 10^7$	5809	
R43	R111†*	$Fe^{2+} + HSO_5^- \rightarrow [Fe(OH)]^{2+} + SO_4^-$	$3 \cdot 10^4$		
R44	R112*	$Mn^{2+} + HSO_5^- \rightarrow SO_4^- + Mn^{3+} + OH^-$	$3 \cdot 10^4$		Implemented based on the ISSA studies (AR) (SO_4^- source)
R45	R113*	$Mn^{2+} + SO_5^- (+ H_2O) \rightarrow Mn^{3+} + HSO_5^- + OH^-$	$1 \cdot 10^{10}$		Implemented based on the ISSA (important SO_5^- sink)
R46	R114†*	$Fe^{2+} + SO_4^- (+ H_2O) \rightarrow [Fe(OH)]^{2+} + SO_4^{2-} + H^+$	$4.6 \cdot 10^9$	-2165	
R47	R117†*	$SO_5^- + SO_5^- \rightarrow 2\ SO_4^- + O_2$	$2.2 \cdot 10^8$	2600	
R48	R118†* R122†* E42†*	$SO_5^- + HO_2 \rightarrow HSO_5^- + O_2$	$1.7 \cdot 10^9$		Explicitly described in the ISSA mechanism
R49	R123†*	$SO_3^- + O_2 \rightarrow SO_5^-$	$2.5 \cdot 10^9$		
R50	R126*	$SO_5^- + SO_3^{2-} (+ H^+) \rightarrow HSO_5^- + SO_3^-$	$2.13 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R51	R127*	$SO_5^- + SO_3^{2-} \rightarrow SO_4^- + SO_4^{2-}$	$5.5 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R52	R128*	$OH + HSO_4^- \rightarrow H_2O + SO_4^-$	$3.5 \cdot 10^5$		Implemented based on the ISSA studies (AR) (main S(VI) sink)
R53	R130*	$SO_4^- + HSO_3^- \rightarrow SO_4^{2-} + SO_3^- + H^+$	$5.8 \cdot 10^8$		Implemented based on the ISSA studies (AR) (important SO_4^- sink)

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n} s^{-1}$	E_a / R, K	Comment
R54	R134*	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	$1.7 \cdot 10^7$		Implemented based on the ISSA studies (AR) (important SO_4^- sink)
R55	R140†	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	11	1110	Implemented based on the non-permanent cloud MR studies (important SO_4^- sink)
	R141†	$HSO_5^- + HSO_3^- + H^+ \rightarrow 2\ SO_4^{2-} + 3\ H^+$	$7.14 \cdot 10^6$		Removed based on the ISSA studies (AR) (minor S(VI) source)
R56	R144†*	$HNO_4 + HSO_3^- \rightarrow HSO_4^- + NO_3^- + H^+$	$3.3 \cdot 10^5$		
		Organic Chemistry			
		Oxidation of Methanol			
R57	R150†* R156†*	$CH_3OH + OH \rightarrow H_2O + O_2CH_2OH - O_2$	$1.0 \cdot 10^9$	580	Explicitly described in the ISSA mechanism
R58	R158†	$O_2CH_2OH + O_2CH_2OH \rightarrow CH_3OH + 2\ O_2 + HCHO$	$1.05 \cdot 10^9$		In reduction step 3c lumped with the reaction above
R59	R157*	$O_2CH_2OH + OH^- \rightarrow HCHO + H_2O + O_2^-$	$1.65 \cdot 10^{10}$		Implemented based on the ISSA studies (AR) (important pathway beside the HO_2 elimination)
		Oxidation of Ethanol			
R60	R159†* R165†*	$CH_3CH_2OH + OH + O_2 \rightarrow H_2O + O_2CH_3CHOH$	$2.1 \cdot 10^9$	1200	Explicitly described in the ISSA mechanism
R61	R166†*	$O_2CH_3CHOH \rightarrow CH_3CHO + HO_2$	52	7217	
R62	R167*	$O_2CH_3CHOH + OH^- \rightarrow CH_3CHO + H_2O + O_2^-$	$8 \cdot 10^9$		Implemented based on the ISSA studies (AR) (important pathway beside the HO_2 elimination)
		Oxidation of Formaldehyde			
R63	R168†* R174†*	$CH_2(OH)_2 + OH + O_2 \rightarrow H_2O + HO_2 + HCOOH$	$1.0 \cdot 10^9$	1020	Explicitly described in the ISSA mechanism
		Oxidation of Acetaldehyde			
R64	R175†* R250†*	$CH_3CH(OH)_2 + OH \rightarrow H_2O + CH_3C(OH)_2O_2 - O_2$	$1.2 \cdot 10^9$		Explicitly described in the ISSA mechanism
R65	R176†* R248†*	$CH_3CHO + OH \rightarrow H_2O + CH_3C(O)O_2 - O_2$	$3.6 \cdot 10^9$		Explicitly described in the ISSA mechanism
		Oxidation of Formic acid			
R66	R187†* R198†*	$HCOOH + OH + O_2 \rightarrow H_2O + CO_2 + HO_2$	$1.3 \cdot 10^8$	1000	Explicitly described in the ISSA mechanism

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n} s^{-1}$	E_a / R, K	Comment
R67	R188†* R198†*	$HCOO^- + OH + O_2 \rightarrow OH^- + CO_2 + HO_2$	$3.2 \cdot 10^9$	1000	Explicitly described in the ISSA mechanism
		Oxidation of Methyl/Ethyl peroxide			
R68	R212†* R213†*	$CH_3O_2 + CH_3O_2 \rightarrow 0.67\ CH_3OH + 0.67\ HCHO + 0.66\ O_2CH_2OH + 0.34\ O_2$	$1.1\ 10^8$		Explicitly described in the ISSA mechanism
R69	R214†*	$CH_3C(O)O_2 + CH_3C(O)O_2 \rightarrow 2\ CH_3O_2 + 2\ CO_2 - O_2$	$1.5 \cdot 10^8$		
R70	R215†*	$CH_3O_2 + HSO_3^- \rightarrow CH_3OOH + SO_3^-$	$5 \cdot 10^5$		
R71	R217†* R216*	$CH_3CH_2O_2 + CH_3CH_2O_2 \rightarrow 0.375\ CH_3CH_2OH + 0.375\ CH_3CHO + 1.25\ CH_3CHOH(O_2) - 0.25\ O_2$	$1.6 \cdot 10^8$	-750	R216 implemented based on the ISSA studies (AR) and lumped with R217
R72	R220*	$Fe^{2+} + CH_3O_2 \rightarrow FeCH_3O_2^{2+}$	$8.6 \cdot 10^5$		Implemented based on the ISSA studies (AR) (important for the TMI processing)
R73	R221*	$FeCH_3O_2^{2+} + H^+ \rightarrow Fe^{3+} + O_2$	$3.0 \cdot 10^4$		Implemented based on the ISSA studies (AR) (important for the TMI processing)
R74	R222*	$FeCH_3O_2^{2+} \rightarrow Fe^{3+} + CH_3OOH + OH^-$	100		Implemented based on the ISSA studies (AR) (important for the TMI processing)
		Oxidation of Oxalic acid			
R75	R223†* R233†*	$OH + HC_2O_4^- + O_2 \rightarrow H_2O + CO_2 + CO_2 + O_2^-$	$1.9 \cdot 10^8$	2800	Explicitly described in the ISSA mechanism
R76	R224* R233*	$NO_3 + HC_2O_4^- \rightarrow NO_3^- + H^+ + CO_2 + CO_2 + O_2^-$	$6.8 \cdot 10^7$		Implemented based on the ISSA studies (AR) and lumped with R233, Explicitly described in the ISSA mechanism (important oxalate sink during the night)
R77	R228†* R233†*	$OH + C_2O_4^{2-} + O_2 \rightarrow OH^- + CO_2 + CO_2 + O_2^-$	$1.6 \cdot 10^8$	4300	Explicitly described in the ISSA mechanism
		Oxidation of Glyoxal			
R78	R234†* R239†* R240†*	$OH + CH(OH)_2CH(OH)_2 + O_2 \rightarrow H_2O + HO_2 + CH(OH)_2COOH$	$1.1 \cdot 10^9$	1516	Explicitly described in the ISSA mechanism
R79	R245* R246* R247*	$SO_4^- + CH(OH)_2CH(OH)_2 \rightarrow H^+ + SO_4^{2-} + HO_2 + CH(OH)_2COOH$	$2.35 \cdot 10^7$	1395	Implemented based on the ISSA studies (AR), Explicitly described in the ISSA mechanism (important glyoxal sink)

N° C3.0RED	N° C2.4	Reaction	k_{298}, $M^{-n} s^{-1}$	E_a / R, K	Comment
R80	R242 R246 R247	$SO_5^- + CH(OH)_2CH(OH)_2 \rightarrow HSO_5^- + + HO_2 + CH(OH)_2COOH$			Implemented based on the non-permanent cloud MR studies (important glyoxal sink)
		Oxidation of Glyoxylic acid			
R81	R241†* R246†* R247†*	$OH + CH(OH)_2COOH + O_2 \rightarrow H_2O + HO_2 + HC_2O_4^- + H^+$	$3.6 \cdot 10^8$	1000	Explicitly described in the ISSA mechanism
R82	R249*	$CH_3C(O)O_2 + O_2^- \rightarrow CH_3C(O)OO^-$	$1 \cdot 10^9$		Implemented based on the ISSA studies (AR)
		Formation of Acetic acid			
R83	R251†*	$CH_3C(OH)_2O_2 \rightarrow 2\ H^+ + CH_3COO^- + O_2^-$	$1 \cdot 10^5$		
R84	R258†*	$CO_2^- + O_2 \rightarrow CO_2 + O_2^-$	$4 \cdot 10^9$		
		Chlorine chemistry			
R85	R262†	$Cl_2^- + Fe^{2+} \rightarrow 2\ Cl^- + Fe^{3+}$	$1.0 \cdot 10^7$	3030	Implemented based on the non-permanent cloud MR studies (important Cl_2^- sink)
R86	R263*	$Cl_2^- + Mn^{2+} \rightarrow MnCl_2^+$	$2 \cdot 10^7$	4090	Implemented based on the ISSA studies (AR)
R87	R264* R265*	$MnCl_2^+ \rightarrow 0.588\ Mn^{2+} + 0.588\ Cl_2^- + 0.412\ Mn^{3+} + 0.824\ Cl^-$	$5.1 \cdot 10^5$		Implemented based on the ISSA studies (AR)
R88	R272†	$Cl_2^- + HSO_3^- \rightarrow 2\ Cl^- + H^+ + SO_3^-$	$1.7 \cdot 10^8$	400	Implemented based on the non-permanent cloud MR studies
R89	R274†	$Cl_2 + H_2O \rightarrow H^+ + Cl^- + HOCl$	0.4	7900	Implemented based on the non-permanent cloud MR studies (important Cl_2 sink)
R90	R275†*	$Cl_2^- + H_2O \rightarrow H^+ + 2\ Cl^- + OH$	23.4		
		Bromine chemistry			
R91	R280†	$Br_2^- + Mn^{2+} \rightarrow MnBr_2^+$	$6.3 \cdot 10^6$	4330	Implemented based on the ISSA studies (AR)
R92	R281† R282†	$MnBr_2^+ \rightarrow 0.577\ Br_2^- + 0.577\ Mn^{2+} + 0.846\ Br^- + 0.423\ Mn^{3+}$	$5.2 \cdot 10^5$		Implemented based on the ISSA studies (AR), Explicitly described in the ISSA mechanism

B- Aqueous phase photolysis reactions:

N° C3.RED	N° C2.4	Reaction	j_{max} [s^{-1}]	Quantum Yield Φ	Comment
R93	R314†*	$H_2O_2 + h\upsilon \rightarrow 2\ OH$	$7.19 \cdot 10^{-6}$	0.98 ± 0.03[a] 0.96 ± 0.03[b]	
R94	R315†	$[Fe(OH)]^{2+} + h\upsilon \rightarrow Fe^{2+} + OH$	$4.51 \cdot 10^{-3}$	0.312 ± 0.03 ... 0.074 ± 0.015[c]	Implemented based on the non-permanent cloud MR studies (important OH source)
R95	R319†*	$NO_3^- + h\upsilon\ (+ H^+) \rightarrow NO_2 + OH$	$4.28 \cdot 10^{-7}$	0.017 ± 0.003	
R96	R320†*	$[Fe(C_2O_4)_2]^- + h\upsilon \rightarrow Fe^{2+} + C_2O_4^{2-} + CO_2 + CO_2^-$	$2.47 \cdot 10^{-2}$	1.0 ± 0.25 (436 nm)	
R97	R321*	$[Fe(C_2O_4)_3]^{3-} + h\upsilon \rightarrow Fe^{2+} + 2\ C_2O_4^{2-} + CO_2 + CO_2^-$	$1.55 \cdot 10^{-2}$	0.6 ± 0.46 (436 nm)	Implemented based on the ISSA studies (AR)

Remarks: [a] λ = 308 nm, T = 298 K; [b] λ = 351 nm, T = 298 K; [c] λ = 280 ... 370 nm; [d] λ= 290...365 nm

C- Aqueous phase equilibriums:

N° C3.0RED	N° C2.4	Reactions	K, M	$k_{298,(for)}$ $M^{-n}\ s^{-1}$	E_a/R, K	$k_{298,(back)}$ $M^{-n}\ s^{-1}$	E_a/R, K	Comment
E1	E1*†	$H_2O \rightleftharpoons H^+ + OH^-$	$1.8 \cdot 10^{-16}$	$2.34 \cdot 10^{-5}$	6800	$1.3 \cdot 10^{11}$		
E2	E2*†	$CO_2 + H_2O \rightleftharpoons H^+ + HCO_3^-$	$4.3 \cdot 10^{-7}$	$2.4 \cdot 10^{-2}$	913	$5.6 \cdot 10^{4}$		
	E3†	$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$	$4.69 \cdot 10^{-11}$	2.35	1820	$5 \cdot 10^{10}$		Removed due to the large pK_a value
E3	E4*†	$HCl \rightleftharpoons H^+ + Cl^-$	$1.72 \cdot 10^{6}$	$5 \cdot 10^{11}$	-6890	$2.9 \cdot 10^{5}$		
E4	E5*†	$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-$	$3.17 \cdot 10^{-7}$	$6.02 \cdot 10^{5}$	560	$3.4 \cdot 10^{10}$		
E5	E6*†	$HO_2 \rightleftharpoons H^+ + O_2^-$	$1.6 \cdot 10^{-5}$	$8.0 \cdot 10^{5}$	0	$5 \cdot 10^{10}$	0	
E6	E7*†	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	22	$1.1 \cdot 10^{12}$	-1800	$5 \cdot 10^{10}$		
E7	E8*†	$HNO_2 \rightleftharpoons H^+ + NO_2^-$	$5.3 \cdot 10^{-4}$	$2.65 \cdot 10^{7}$	1760	$5 \cdot 10^{10}$		
E8	E9*†	$HNO_4 \rightleftharpoons H^+ + O_2NO_2^-$	$1 \cdot 10^{-5}$	$5 \cdot 10^{5}$		$5 \cdot 10^{10}$		
E9	E10*†	$NO_2 + HO_2 \rightleftharpoons HNO_4$	$2.2 \cdot 10^{9}$	$1.0 \cdot 10^{7}$		$4.6 \cdot 10^{-3}$		
E10	E11*†	$SO_2 + H_2O \rightleftharpoons HSO_3^- + H^+$	$3.13 \cdot 10^{-4}$	$6.27 \cdot 10^{4}$	-1940	$2.0 \cdot 10^{8}$		
E11	E12*†	$HSO_3^- \rightleftharpoons SO_3^{2-} + H^+$	$6.22 \cdot 10^{-8}$	3110	-1960	$5 \cdot 10^{10}$		

N° C3.0RED	N° C2.4	Reactions	K, M	$k_{298,(for)}$ $M^{-n}\ s^{-1}$	E_a/R, K	$k_{298,(back)}$ $M^{-n}\ s^{-1}$	E_a/R, K	Comment
E12	E13*†	$H_2SO_4 \rightleftharpoons HSO_4^- + H^+$	1000	$5\cdot10^{13}$		$5\cdot10^{10}$		
E13	E14*†	$HSO_4^- \rightleftharpoons SO_4^{2-} + H^+$	$1.02\cdot10^{-2}$	$1.02\cdot10^{9}$	-2700	$1\cdot10^{11}$		
E14	E15*†	$HCOOH \rightleftharpoons HCOO^- + H^+$	$1.77\cdot10^{-4}$	$8.85\cdot10^{6}$	-12	$5\cdot10^{10}$		
E15	E16*†	$CH_3COOH \rightleftharpoons CH_3COO^- + H^+$	$1.75\cdot10^{-5}$	$8.75\cdot10^{5}$	-46	$5\cdot10^{10}$		
E16	E17*†	$Fe^{3+} + H_2O \rightleftharpoons [Fe(OH)]^{2+} + H^+$	$1.1\cdot10^{-4}$	$4.7\cdot10^{4}$		$4.3\cdot10^{8}$		
E17	E18†	$[Fe(OH)]^{2+} + H_2O \rightleftharpoons [Fe(OH)_2]^+ + H^+$	$1.4\cdot10^{-7}$	$1.1\cdot10^{3}$		$8.0\cdot10^{9}$		Implemented based on the ISSA studies (AR)
E18	E20*†	$HCHO + H_2O \rightleftharpoons CH_2(OH)_2$	36	0.18	-4030	$5.1\cdot10^{-3}$		
E19	E21*†	$CH_3CHO + H_2O \rightleftharpoons CH_3CH(OH)_2$	$2.46\cdot10^{-2}$	$1.4\cdot10^{-4}$	-2500	$5.69\cdot10^{-3}$		
E20	E22*†	$HCHO + HSO_3^- \rightleftharpoons HMS^- + H_2O$	$6.6\cdot10^{9}$	$7.9\cdot10^{2}$	3293	$1.2\cdot10^{-7}$	5831	Implemented based on the non-permanent cloud MR studies
E21	E23*†	$HCHO + SO_3^{2-} + (H_2O) \rightleftharpoons HMS^- + OH^-$	$6.6\cdot10^{9}$	$2.5\cdot10^{7}$	2752	$3.79\cdot10^{-3}$	5290	
E22	E24*†	$Cl + Cl^- \rightleftharpoons Cl_2^-$	$1.4\cdot10^{5}$	$8.5\cdot10^{9}$		$6\cdot10^{4}$		
E23	E25†	$Br + Br^- \rightleftharpoons Br_2^-$	$6\cdot10^{5}$	$1.2\cdot10^{10}$		$1.9\cdot10^{4}$		Implemented based on the ISSA studies (AR)
E24	E26*†	$Cl^- + OH \rightleftharpoons ClOH^-$	0.7	$4.3\cdot10^{9}$		$6.1\cdot10^{9}$		
E25	E27*†	$ClOH^- + H^+ \rightleftharpoons Cl + H_2O$	$5.1\cdot10^{6}$	$2.1\cdot10^{10}$		4100		
E26	E28†	$ClOH^- + Cl^- \rightleftharpoons Cl_2^- + OH^-$	$2.2\cdot10^{-4}$	$1.0\cdot10^{4}$		$4.5\cdot10^{7}$		Implemented based on the ISSA studies (AR)
E27	E29†	$Br^- + OH \rightleftharpoons BrOH^-$	333	$1.1\cdot10^{10}$		$3.3\cdot10^{7}$		Implemented based on the ISSA studies (AR)
E28	E30†	$BrOH^- + H^+ \rightleftharpoons Br + H_2O$	$1.8\cdot10^{12}$	$4.4\cdot10^{10}$		$2.45\cdot10^{-2}$		Implemented based on the ISSA studies (AR)
E29	E31†	$BrOH^- + Br^- \rightleftharpoons Br_2^- + OH^-$	70	$1.9\cdot10^{8}$		$2.7\cdot10^{6}$		Implemented based on the ISSA studies (AR)
E30	E32†	$Mn^{3+} + H_2O \rightleftharpoons Mn(OH)^{2+} + H^+$	0.93	$1.86\cdot10^{10}$		$2.0\cdot10^{10}$		Implemented based on the ISSA studies (AR)
E31	E33†	$O_2^- + Mn^{2+} \rightleftharpoons MnO_2^+$	$2.3\cdot10^{4}$	$1.5\cdot10^{8}$		$6.5\cdot10^{3}$		Implemented based on the ISSA studies (AR)
E32	E34†	$HO_2 + Mn^{2+} \rightleftharpoons MnO_2^+ + H^+$	0.17	$1.1\cdot10^{6}$		$6.5\cdot10^{6}$		Implemented based on the ISSA studies (AR)
E33	E36†	$Mn(OH)^{2+} + H_2O \rightleftharpoons Mn(OH)_2^+ + H^+$	$1\cdot10^{-5}$	$2\cdot10^{5}$		$2\cdot10^{10}$		Implemented based on the ISSA studies (AR)
E34	E39*†	$HO_3 \rightleftharpoons H^+ + O_3^-$	$5\cdot10^{-9}$	330		$5.2\cdot10^{10}$		
	E41†	$CHOHSO_3^- \rightleftharpoons CHOSO_3^{2-} + H^+$	$1.34\cdot10^{-6}$	$5.9\cdot10^{4}$		$4.4\cdot10^{10}$		Removed based on the non-permanent cloud MR studies
	E42†	$SO_5O_2H^- \rightleftharpoons SO_5O_2^{2-} + H^+$	$1.5\cdot10^{-5}$	$7.5\cdot10^{5}$		$5\cdot10^{10}$		Removed due to the lumping of the whole reaction chain

N° C3.0RED	N° C2.4	Reactions	K, M	$k_{298,(for)}$ M^{-n} s^{-1}	E_a/R, K	$k_{298,(back)}$ M^{-n} s^{-1}	E_a/R, K	Comment
	E43†	$H_2C_2O_4 \rightleftharpoons H^+ + HC_2O_4^-$	$6.4\cdot10^{-2}$	$3.2\cdot10^{9}$		$5\cdot10^{10}$		Removed based on the non-permanent cloud MR studies
E35	E44*†	$HC_2O_4^- \rightleftharpoons H^+ + C_2O_4^{2-}$	$6.25\cdot10^{-5}$	$2.6\cdot10^{6}$		$5\cdot10^{10}$		
E36	E45*†	$CH(OH)_2COOH \rightleftharpoons H^+ + CH(OH)_2COO^-$	$3.16\cdot10^{-4}$	$6.32\cdot10^{6}$		$2\cdot10^{10}$		
	E46†	$CHOCHO + H_2O \rightleftharpoons CH(OH)_2CH(OH)_2$	$3.9\cdot10^{3}$	21.5		$5.5\cdot10^{-3}$		Removed based on the non-permanent cloud studies (MR) (effective hydration, thus implemented as effective uptake with the direct formation of the hydrate)
E37	E47*†	$[Fe(C_2O_4)]^+ \rightleftharpoons [Fe]^{3+} + C_2O_4^{2-}$	$2.9\cdot10^{9}$	$3\cdot10^{-3}$		$7.5\cdot10^{6}$		
E38	E48*†	$[Fe(C_2O_4)_2]^- \rightleftharpoons [Fe(C_2O_4)]^+ + C_2O_4^{2-}$	$6.3\cdot10^{6}$	$3\cdot10^{-3}$		$1.89\cdot10^{4}$		
E39	E49†	$[Fe(C_2O_4)_3]^{3-} \rightleftharpoons [Fe(C_2O_4)_2]^- + C_2O_4^{2-}$	$3.8\cdot10^{4}$	$3\cdot10^{-3}$		38		
E40	E50*†	$SO_4^- + Cl^- \rightleftharpoons SO_4^{2-} + Cl$	1.2	$2.52\cdot10^{8}$		$2.1\cdot10^{8}$		
E41	E51*†	$NO_3 + Cl^- \rightleftharpoons NO_3^- + Cl$	3.4	$3.4\cdot10^{8}$		$1\cdot10^{8}$		
E42	E53†	$CH_3C(O)OOH \rightleftharpoons CH_3C(O)OO^- + H^+$	$6.3\cdot10^{-9}$	315		$5\cdot10^{10}$		Implemented based on the ISSA studies (AR)
	E54†	$CH_3CO + H_2O \rightleftharpoons CH_3C(OH)_2$	$1.2\cdot10^{-2}$	$2\cdot10^{4}$		$3\cdot10^{4}$		Removed based on the non-permanent cloud studies (MR) (effective hydration, thus implemented as effective uptake with the direct formation of the hydrate)

Remarks: † Reaction considered in the ISSA mechanism [C3.0ISSARED(Aut)]; * Reaction considered in the manually reduced CAPRAM mechanism [C3.0CondRED(Man)]

D- Aqueous phase reactions (organic extension):

N° C3.0RED	N° C3.0	Reaction	$k_{298\,K}$ $[M^{-1}\,s^{-1}]$	$-E_A/R$ [K]	Comment
		Oxidation of glyoxylate (hydrated form)			
R98	R1, R3	$OH + CH(OH)_2COO^- + O_2 \rightarrow H_2O + O_2C(OH)_2COO^-$	$2.6\cdot10^{9}$	4300	[a]

N° C3.0RED	N° C3.0	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comment
R99	R4-R7	$2\ O_2C(OH)_2COO^- \rightarrow 1.31\ CO_2^- + 2.69\ CO_2 + 0.9\ H_2O_2 + 0.58\ OH^- + 0.81\ H_2O + 0.29\ O_2 + 0.11\ O_2^-$	$6.55\cdot10^7$		[a]
		Oxidation of methylglyoxal (hydrated form)			
R100	R50, R52 R53	$CH_3C(O)CH(OH)_2 + OH + O_2 \rightarrow CH_3C(O)COOH + HO_2 + H_2O$	$7.9\cdot10^8$	1589	[a]
R101	R51-R53	$NO_3 + CH_3C(O)CH(OH)_2 + O_2 \rightarrow CH_3C(O)COOH + HO_2 + NO_3^- + H^+$	$6.3\cdot10^7$		[a]
		Oxidation of pyruvic acid			
R102	R75, R77-R81	$OH + CH_3C(O)COOH + 0.625\ O_2 + 0.115\ OH^- + 0.565\ OHCC(O)COOH + 0.145\ CH_2OHC(O)COOH + 0.3\ H_2O_2 + 0.29\ CO_2 + 0.115\ O_2^- + 0.29\ CH_3CHO + 0.825\ H_2O$	$1.2\cdot10^8$	2800	[a]
		Oxidation of pyruvate			
R103	R82, R84-R88	$CH_3C(O)COO^- + OH + 0.625\ O_2 \rightarrow 0.565\ OHCC(O)COO^- + 0.145\ CH_2OHC(O)COO^- + 0.3\ H_2O_2 + 0.29\ CH_3CHO + 0.29\ CO_2 + 0.175\ OH^- + 0.115\ O_2^- + 0.535\ H_2O$	$7\cdot10^8$	2285	[a]
R104	R83-R88	$NO_3 + CH_3C(O)COO^- + 0.625\ O_2 + 0.29\ H_2O \rightarrow 0.565\ OHCC(O)COO^- + 0.145\ CH_2OHC(O)COO^- + 0.3\ H_2O_2 + 0.29\ CH_3CHO + 0.29\ CO_2 + 0.115\ O_2^- + NO_3^- + 0.825\ H^+$	$1.9\cdot10^8$		[a]
		Oxidation of glycolic acid			
R105	R126, R128-R129	$CH_2OHCOOH + OH + O_2 \rightarrow HO_2 + CH(OH)_2COOH$	$5.4\cdot10^8$		[a]
		Oxidation of glycolate			
R106	R130, R132-R133	$CH_2OHCOO^- + OH + O_2 \rightarrow HO_2 + CH(OH)_2COO^-$	$1.2\cdot10^9$		[a]
R107	R131-R133	$NO_3 + CH_2OHCOO^- + O_2 \rightarrow HO_2 + CH(OH)_2COO^- + NO_3^- + H^+ - H_2O$	$1.1\cdot10^9$		[a]
		Oxidation of 1,4-butenedial			
R108	R205-R207	$OH + OHCCH{=}CHCHO + 0.5\ O_2 \rightarrow 0.5\ OHCCH(OH)C(O)CHO + 0.5\ OHCCH(OH)CH(OH)CHO$	$6\cdot10^9$		[a]
		Oxidation of 2-hydroxy, 3,4-dioxo butyraldehyde			
R109	R208, R210-R211	$OHCCH(OH)C(O)CHO + OH + O_2 \rightarrow HOOCCH(OH)C(O)CHO + HO_2 - H_2O$	$1.1\cdot10^9$	1516	[a]

N° C3.0RED	N° C3.0	Reaction	$k_{298\ K}$ [$M^{-1}\ s^{-1}$]	- E_A/R [K]	Comment
		Oxidation of 2-hydroxy, 3,4-dioxo butyric acid			
R110	R212, R214-R215	$HOOCCH(OH)C(O)CHO + OH + O_2 \rightarrow HOOCC(O)CH(OH)COOH + HO_2$	$3.6\cdot10^8$	1000	[a]
R111	R213-R215	$HOOCCH(OH)C(O)CHO + NO_3 + O_2 \rightarrow HOOCC(O)CH(OH)COOH + HO_2 + NO_3^- + H^+ - H_2O$	$3.4\cdot10^6$		[b] Considered based on the non-permanent cloud MR studies
R112	R216	$HOOCC(O)CH(OH)COOH \rightarrow CO_2 + CH_2OHC(O)COOH$	$1\cdot10^{-5}$		
		Oxidation of 2-hydroxy, 3,4-dioxo butyrate			
R113	R217, R219-R220	$^-OOCCH(OH)C(O)CHO + OH + O_2 \rightarrow HOOCC(O)CH(OH)COO^- + HO_2$	$2.6\cdot10^9$	4300	[a]
R114	R221	$HOOCC(O)CH(OH)COO^- \rightarrow CO_2 + CH_2OHC(O)COO^-$	$1\cdot10^{-5}$		
R115		**Oxidation of 2,3-dihydroxy, 4-oxo butyraldehyde**			
R116	R222, R224-R225	$OHCCH(OH)CH(OH)CHO + OH + O_2 \rightarrow HOOCCH(OH)CH(OH)CHO + HO_2$	$1.1\cdot10^9$	1516	[a]
R117	R223-R225	$OHCCH(OH)CH(OH)CHO + NO_3 + O_2 \rightarrow HOOCCH(OH)CH(OH)CHO + HO_2 + NO_3^- + H^+ - H_2O$	$6\cdot10^6$		[b] Considered based on the non-permanent cloud MR studies
		Oxidation of 2,3-dihydroxy, 4-oxo butyric acid			
R118	R226, R228-R229	$HOOCCH(OH)CH(OH)CHO + OH + O_2 \rightarrow HOOCCH(OH)CH(OH)COOH + HO_2$	$3.6\cdot10^8$	1700	[a]
R119	R227-R229	$HOOCCH(OH)CH(OH)CHO + NO_3 + O_2 \rightarrow HOOCCH(OH)CH(OH)COOH + HO_2 + NO_3^- + H^+ - H_2O$	$6\cdot10^6$		[b] Considered based on the non-permanent cloud MR studies
		Oxidation of 2,3-dihydroxy, 4-oxo butyrate			
R120	R230; R232-R233	$^-OOCCH(OH)CH(OH)CHO + OH + O_2 \rightarrow {}^-OOCCH(OH)CH(OH)COOH + HO_2$	$9.7\cdot10^8$	1575	[a]
R121	R231-R233	$^-OOCCH(OH)CH(OH)CHO + NO_3 + O_2 \rightarrow {}^-OOCCH(OH)CH(OH)COOH + HO_2 + NO_3^- + H^+ - H_2O$	$1.2\cdot10^9$		[a]
		Oxidation of ethylene glycol			
R122	R234, R236-R237	$CH_2OHCH_2OH + OH + O_2 \rightarrow OHCCH_2OH + HO_2 + H_2O$	$1.4\cdot10^9$		[a]
		Oxidation of glycolaldehyde			
R123	R238, R240-R241	$OHCCH_2OH + OH + O_2 \rightarrow CH_2OHCOOH + HO_2$	$3.6\cdot10^9$		[a]

N° C3.0RED	N° C3.0	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	$-E_A/R$ [K]	Comment
		Oxidation of glycolaldehyde (hydrated form)			
R124	R242, R244-R245	$(OH)_2CHCH_2OH + OH + O_2 \rightarrow CH_2OHCOOH + HO_2$	$1.2\cdot10^9$		[a]
R125	R243-R245	$(OH)_2CHCH_2OH + NO_3 + O_2 \rightarrow CH_2OHCOOH + HO_2 + NO_3^- + H^+$	$1.1\cdot10^7$		[b] Considered based on the non-permanent cloud MR studies
		Oxidation of 3-hydroxy pyruvic acid			
R126	R246, R248-R249	$CH_2OHC(O)COOH + OH + O_2 \rightarrow OHCC(O)COOH + HO_2 + H_2O$	$5.4\cdot10^8$		[a]
R127	R250	$OHCC(O)COOH + H_2O \rightarrow CH_3CHO + CO_2 + O_2$	$1\cdot10^{-5}$		
		Oxidation of 3-hydroxy pyruvate			
R128	R251, R253-R254	$CH_2OHC(O)COO^- + OH + O_2 \rightarrow OHCC(O)COO^- + HO_2 + H_2O$	$1.2\cdot10^9$		[a]
R129	R252-R254	$CH_2OHC(O)COO^- + NO_3 + O_2 \rightarrow OHCC(O)COO^- + HO_2 + NO_3^- + H^+$	$1.8\cdot10^9$		[a]
R130	R255	$OHCC(O)COO^- + H_2O \rightarrow CH(OH)_2CH(OH)_2 + CO_2 + OH^-$	$1\cdot10^{-6}$		
		Oxidation of 3-oxo, pyruvic acid			
R131	R256, R258-R259	$OHCC(O)COOH + OH + O_2 \rightarrow HOOCC(O)COOH + HO_2$	$3.6\cdot10^8$	1000	[a]
		Oxidation of 3-oxo, pyruvate			
R132	R260, R262-R263	$OHCC(O)COO^- + OH + O_2 \rightarrow HOOCC(O)COO^- + HO_2$	$2.6\cdot10^9$	4300	[a]
R133	R261-R263	$OHCC(O)COO^- + NO_3 + O_2 \rightarrow HOOCC(O)COO^- + HO_2 + NO_3^- + H^+ - H_2O$	$9.3\cdot10^9$		[a]
		Decarboxylation of 2-hydroxy, 3-oxo succinic acid/succinate			
R134	R277	$HOOCC(O)CH(OH)COOH \rightarrow CO_2 + OHCCH(OH)COOH$	$1\cdot10^{-5}$		
R135	R287	$HOOCC(O)CH(OH)COO^- \rightarrow CO_2 + OHCCH(OH)COO^-$	$1\cdot10^{-6}$		
		Oxidation of 3-oxo, lactic acid			
R136	R278, R280-R281	$OH + OHCCH(OH)COOH + O_2 \rightarrow OHCC(O)COOH + HO_2 + H_2O$	$4.3\cdot10^8$		[a]
R137	R279-R281	$NO_3 + OHCCH(OH)COOH + O_2 \rightarrow OHCC(O)COOH + HO_2 + NO_3^- + H^+$	$3\cdot10^6$		[b] Considered based on the non-permanent cloud MR studies
		Oxidation of 3-oxo, lactate			

N° C3.0RED	N° C3.0	Reaction	$k_{298\,K}$ [$M^{-1}\,s^{-1}$]	- E_A/R [K]	Comment
R138	R288, R290-R291	$OH + OHCCH(OH)COO^- + O_2 \rightarrow OHCC(O)COO^- + HO_2 + H_2O$	$1.2\cdot10^9$		[a]
R139	R289-R291	$NO_3 + OHCCH(OH)COO^- + O_2 \rightarrow OHCC(O)COO^- + HO_2 + NO_3^- + H^+$	$5.4\cdot10^9$		[a]
		Decarboxylation of ketomalonic acid			
R140	R296	$HOOCC(O)COOH + H_2O \rightarrow CO_2 + CH(OH)_2COOH$	$1\cdot10^{-5}$		
R141	R301	$HOOCC(O)COO^- + H_2O \rightarrow CO_2 + CH(OH)_2COO^-$	$1\cdot10^{-6}$		
R142	R336	$2\ CH_3CH(OO)OH \rightarrow H_2O_2 + 2\ CH_3COOH$	$3.5\cdot10^8$		
		HO_2 elimination from $CH_3C(OH)_2O_2$			
R143	R362	$CH_3C(OH)_2O_2 \rightarrow CH_3COOH + HO_2$	1000		

Remarks: The above-presented reactions are considered in both the ISSA mechanism [C3.0ISSARED(Aut)] and the manually reduced CAPRAM mechanism [C3.0condRED(Man)]. Exceptions are marked with a comment. Moreover, the oxidations of 2-propanol, acetone, hydroxy acetone and methyl ethyl ketone, which are considered in the ISSA mechanism, are not presented in the table and have been also not considered in the final reduced mechanism due to their minor chemical importance.
[a] Reactions explicitly described in their elementary steps in the ISSA mechanism [C3.0ISSARED(Aut)]; [b] Reaction removed in the ISSA mechanism [C3.0ISSARED(Aut)]

E- Aqueous phase equilibriums (organic extension):

N° C3.0RED	N° C3.0	Equilibrium	K	Ea/R	k_{for}	k_{back}	comment
E43	E2†*	$CH_3C(O)COOH \rightleftharpoons H^+ + CH_3C(O)COO^-$	$3.55\cdot10^{-3}$		$1.8\cdot10^8$	$5\cdot10^{10}$	
E44	E8†*	$CH_2OHCOOH \rightleftharpoons CH_2OHCOO^- + H^+$	$1.48\cdot10^{-4}$		$7.4\cdot10^6$	$5\cdot10^{10}$	
	E3†	$CH_3C(O)CHO + H_2O \rightleftharpoons CH_3C(O)CH(OH)_2$	48.6		21.5	0.543	Removed based on the non-permanent cloud studies (MR) (effective hydration, thus implemented as effective uptake with the direct formation of the hydrate)
E45	E10†*	$CH_3C(O)O_2 + H_2O \rightleftharpoons CH_3C(OH)_2O_2$	367		$1.1\cdot10^7$	$3\cdot10^4$	
E46	E12†*	$HOOCCH(OH)C(O)CHO \rightleftharpoons {}^-OOCCH(OH)C(O)CHO + H^+$	$4.57\cdot10^{-5}$		$2.29\cdot10^6$	$5\cdot10^{10}$	

N° C3.0RED	N° C3.0	Equilibrium	K	Ea/R	k_{for}	k_{back}	comment
E47	E13†*	$HOOCC(O)CH(OH)COOH \rightleftharpoons HOOCC(O)CH(OH)COO^- + H^+$	$6.03 \cdot 10^{-3}$		$3.01 \cdot 10^{8}$	$5 \cdot 10^{10}$	
E48	E14†*	$CH_2OHC(O)COOH \rightleftharpoons CH_2OHC(O)COO^- + H^+$	$3.55 \cdot 10^{-3}$		$1.8 \cdot 10^{8}$	$5 \cdot 10^{10}$	
E49	E15†*	$HOOCCH(OH)CH(OH)CHO \rightleftharpoons {}^-OOCCH(OH)CH(OH)CHO + H^+$	$4.57 \cdot 10^{-5}$		$2.29 \cdot 10^{6}$	$5 \cdot 10^{10}$	
E50	E16†*	$HOOCCH(OH)CH(OH)COOH \rightleftharpoons {}^-OOCCH(OH)CH(OH)COOH + H^+$	$1.05 \cdot 10^{-3}$		$5.25 \cdot 10^{7}$	$5 \cdot 10^{10}$	
E51	E17†*	$OHCC(O)COOH \rightleftharpoons OHCC(O)COO^- + H^+$	$3.55 \cdot 10^{-3}$		$1.8 \cdot 10^{8}$	$5 \cdot 10^{10}$	
E52	E18†*	$HOOCC(O)COOH \rightleftharpoons HOOCC(O)COO^- + H^+$	$3.16 \cdot 10^{-3}$		$1.58 \cdot 10^{8}$	$5 \cdot 10^{10}$	
E53	E28†*	$OHCCH(OH)COOH \rightleftharpoons OHCCH(OH)COO^- + H^+$	$1.35 \cdot 10^{-5}$			$5 \cdot 10^{10}$	
E54	E32†*	$OHCCH_2OH + H_2O \rightleftharpoons (OH)_2CHCH_2OH$	$1.64 \cdot 10^{-1}$		$1.57 \cdot 10^{-3}$	$9.6 \cdot 10^{-3}$	
E55	E35†	$HOOCC(O)COO^- \rightleftharpoons {}^-OOCC(O)COO^- + H^+$	$1.64 \cdot 10^{-4}$		$8.2 \cdot 10^{6}$	$5 \cdot 10^{10}$	Implemented based on the ISSA studies (AR)

Remarks: † Equilibriums considered in the ISSA mechanism [C3.0ISSARED(Aut)]; * Equilibriums considered in the manually reduced CAPRAM mechanism [C3.0condRED(Man)]